

2,2,3,3,4,4,5,5,6,7,7,7-Dodecafluoro-6-(trifluoromethyl)heptanoic acid
15166-06-0 | DTXSID50562865

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 4.97

Global applicability domain: Outside

Local applicability domain index: 1.85e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

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4-Hydroxy-1-naphthalenesulfonic acid monosodium salt

Measured: 12.9

Predicted: 6.33

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1,1,1,3,3,3-Hexafluoro-2-propanol

Measured: 2.51

Predicted: 2.40

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2-Amino-1-naphthalenesulfonic acid

Measured: 6.03

Predicted: 6.40

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Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt

Measured: 3.02

Predicted: 5.14

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Sodium 3-nitrobenzenesulfonate

Measured: 5.01

Predicted: 5.24